

Convergence to equilibrium for smectic-A liquid crystals in 3D domains

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In collaboration: B. Climent-Ezquerro (Univ. Sevilla),

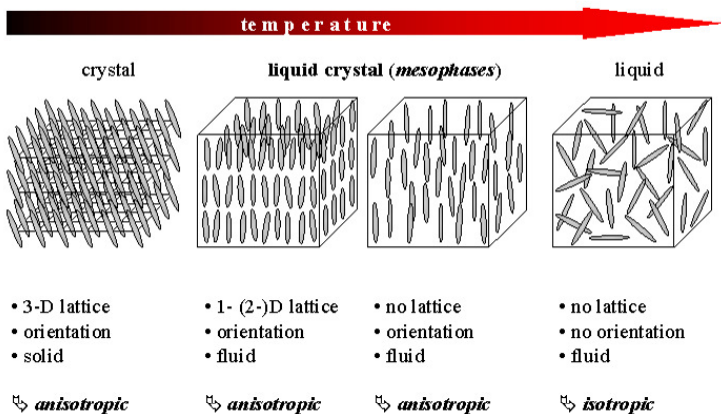
. [NA-TMA'14].

- **Liquid crystals (LC)** exhibit properties between liquids and solids. A **LC** can behave like a liquid (macroscopically), but their molecules have a preferential **orientation** (microscopically), due to **elasticity** effects (**anisotropic liquids**).
- The time-dynamics interaction between **macroscopic** and **microscopic** is modeled by nonlinear parabolic PDE + **gradient flow**, involving:
 - Macroscopic: fluid dynamics (Navier-Stokes)
 - Microscopic: **order parameter**
- Different phases in LC, for instance:
 - **nematic** phases, with orientational order of molecules,
 - **smectic** phases, with moreover positional order (arranged in layers).

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thermotropic liquid crystals



Static Oseen-Frank's theory for nematic LC

- $\Omega \subset \mathbb{R}^d$ ($d = 2, 3$): domain filled by the LC, with boundary $\partial\Omega$
- Equilibrium states: minimum of a free energy
- **Oseen-Frank** free energy derive to the Static (Minimization) problem:

$$\min_{|\mathbf{d}|=1} E_{ela}(\mathbf{d})$$

where E_{ela} is the **elastic** energy functional:

$$E_{ela}(\mathbf{d}) = \int_{\Omega} \left(\frac{k_1}{2} (\nabla \cdot \mathbf{d})^2 + \frac{k_2}{2} (\mathbf{d} \cdot (\nabla \times \mathbf{d}))^2 + \frac{k_3}{2} |\mathbf{d} \times (\nabla \times \mathbf{d})|^2 \right)$$

$k_i > 0$ elastic constants.

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- **Smectic LC**: the molecules have an orientational order vector \mathbf{d} and a positional order (layer structure of normal vector \mathbf{n}). Assume:
 - \exists a potential function φ s.t. layers = level sets of φ :

$$\nabla \times \mathbf{n} = 0 \quad \Longleftrightarrow \quad \mathbf{n} = \nabla \varphi$$

- Incompressibility of the layers: $|\mathbf{n}| = 1$.
- **Smectic-A LC**: Assume $\mathbf{d} = \mathbf{n}$.
- Since $\mathbf{d} = \mathbf{n}$ and $\mathbf{n} = \nabla \varphi$, the elastic energy can be rewritten (reduced form) as

$$E_{ela} = \frac{1}{2} \int_{\Omega} |\nabla \cdot \mathbf{n}|^2 = \frac{1}{2} \int_{\Omega} |\Delta \varphi|^2$$

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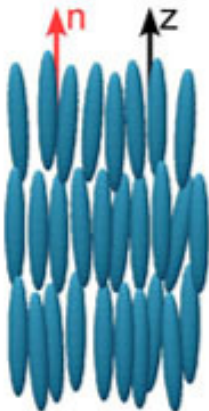
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Nematic
(N)



Smectic A
(SmA)



Smectic C
(SmC)

A static Smectic-A LC problem

- Regularized Oseen-Frank energy (by penalization of **Ginzburg-Landau** type):

$$E_\varepsilon := \int_{\Omega} \left(\frac{1}{2} (\Delta \varphi)^2 + \frac{1}{\varepsilon^2} F(\nabla \varphi) \right), \quad F(\mathbf{n}) = \frac{1}{4} (|\mathbf{n}|^2 - 1)^2$$

Static (Minimization) problem:

$$\min_{\varphi} E_\varepsilon$$

Remark: Problem without constraints but non-convex functional.

- Optimality system:

$$\left\langle \frac{\delta E_\varepsilon(\varphi)}{\delta \varphi}, \bar{\varphi} \right\rangle = \int_{\Omega} \Delta \varphi \Delta \bar{\varphi} + \frac{1}{\varepsilon^2} \mathbf{f}(\nabla \varphi) \cdot \nabla \bar{\varphi} = 0 \quad \forall \bar{\varphi}$$

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- ① Assuming $\Delta\varphi|_{\partial\Omega} = 0$ (N1) or $\nabla\bar{\varphi} \cdot \mathbf{m}|_{\partial\Omega} = 0$ (D2) (\mathbf{m} is the normal vector):

$$\left\langle \frac{\delta E_\theta(\varphi)}{\delta\varphi}, \bar{\varphi} \right\rangle = - \int_{\Omega} \mathbf{w} \cdot \nabla \bar{\varphi}, \quad \mathbf{w} := \nabla \Delta\varphi - \frac{1}{\varepsilon^2} \mathbf{f}(\nabla\varphi).$$

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Admissible B.C. to fourth-order Euler-Lagrange $\nabla \cdot \mathbf{w} = 0$

$$[D1 - D2] \quad \varphi|_{\partial\Omega} = \varphi_1, \quad \nabla\varphi \cdot \mathbf{m}|_{\partial\Omega} = \varphi_2,$$

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$$[N1 - N2] \quad \Delta\varphi|_{\partial\Omega} = 0, \quad \mathbf{w} \cdot \mathbf{m}|_{\partial\Omega} = 0.$$

Non admissible B.C.: $[D1-N2]$ and $[D2-N1]$

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Smectic-A Liquid Crystal Model [E, ARMA'97]

- $\Omega \subset \mathbb{R}^3$, $Q = \Omega \times (0, T)$ and $\Sigma = \partial\Omega \times (0, T)$.
- **Linear momentum**, (\mathbf{u}, p) -system in Q :

$$\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{u} + \nabla p - \nabla \cdot (\sigma^d + \lambda \sigma^e) = 0, \quad \nabla \cdot \mathbf{u} = 0,$$

- $\sigma^d = \sigma^d(D(\mathbf{u}), \mathbf{n})$: dissipative (symmetric) stress tensor:

$$\sigma^d = \mu_1(\mathbf{n}^t D \mathbf{n}) \mathbf{n} \otimes \mathbf{n} + \mu_4 D + \mu_5(D \mathbf{n} \otimes \mathbf{n} + \mathbf{n} \otimes D \mathbf{n}), \quad D = \frac{\nabla \mathbf{u} + \nabla \mathbf{u}^t}{2}$$

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- **Angular momentum**, φ -equation in Q (of Allen-Cahn's type):

$$\frac{\partial \varphi}{\partial t} + \mathbf{u} \cdot \nabla \varphi + \gamma \frac{\delta E_e}{\delta \varphi} = 0,$$

$\gamma > 0$ constant (elastic relaxation time).

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- Initial-boundary problem (with Dirichlet [D1-D2] B.C. for φ) in Q :

$$(P) \quad \left\{ \begin{array}{ll} \frac{D\mathbf{u}}{Dt} - \nabla \cdot \sigma^d + \nabla \tilde{p} - \lambda \frac{\delta E_e}{\delta \varphi} \nabla \varphi &= \mathbf{0}, & \mathbf{u} \\ \nabla \cdot \mathbf{u} &= 0, & p \\ \frac{\partial \varphi}{\partial t} + \mathbf{u} \cdot \nabla \varphi + \gamma \frac{\delta E_e}{\delta \varphi} &= 0, & \frac{\delta E_e}{\delta \varphi} \\ \Delta^2 \varphi - \frac{1}{\varepsilon^2} \nabla \cdot \mathbf{f}(\nabla \varphi) &= \frac{\delta E_e}{\delta \varphi}, & \frac{\partial \varphi}{\partial t} \\ \mathbf{u}|_{\Sigma} = \mathbf{0}, \quad \varphi|_{\Sigma} = \varphi_1, \quad \partial_n \varphi|_{\Sigma} &= \varphi_2, \\ \mathbf{u}|_{t=0} = \mathbf{u}_0, \quad \varphi|_{t=0} &= \varphi_0 \end{array} \right.$$

- $\tilde{p} = p + \lambda E_e$ (Lagrange multiplier \sim constraint $\nabla \cdot \mathbf{u} = 0$)
- Other B.C. are possible. For instance, $\mathbf{w} \cdot \mathbf{m}|_{\partial\Omega} = 0$ implies the conservation property $\frac{d}{dt} \int_{\Omega} \varphi = 0$.

Dissipative Energy law and weak solutions

Testing by $\mathbf{u}, p, \frac{\delta E_e}{\delta \varphi}, \frac{\partial \varphi}{\partial t}$:

$$(EL) \quad \frac{d}{dt} \left(E_{kin}(\mathbf{u}) + \lambda E_e(\varphi) \right) + \int_{\Omega} \sigma^d : D + \lambda \gamma \int_{\Omega} \left| \frac{\delta E_e}{\delta \varphi} \right|^2 = 0$$

where

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$$\sigma^d : D = \mu_1 (\mathbf{n}^t D \mathbf{n})^2 + \mu_4 |D|^2 + \mu_5 |D \mathbf{n}|^2 \geq \mu_4 |D|^2.$$

Weak solutions (variational $\sim (\mathbf{u}, p)$, point-wise $\sim \varphi$):

$$\mathbf{u} \in L^\infty(0, +\infty; \mathbf{L}^2(\Omega)) \cap L^2(0, +\infty; \mathbf{H}^1(\Omega)), \quad \frac{\delta E_e}{\delta \varphi} \in L^2(0, +\infty; L^2(\Omega)).$$

$$\varphi \in L^\infty(0, +\infty; H^2(\Omega)) \cap L^2_{loc}(0, +\infty; H^4(\Omega)), \quad \frac{\partial \varphi}{\partial t} \in L^2(0, +\infty; L^2(\Omega)).$$

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- Combining adequately **\mathbf{u} -system** by **$A\mathbf{u} + \partial_t \mathbf{u}$** and **$\partial_t(\varphi\text{-eq})$** by **$\partial_t \varphi$** :

$$\Phi' + \Psi \leq C(\Phi^3 + 1),$$

$$\Phi(t) := \|\mathbf{u}\|_{H^1}^2 + \|\partial_t \varphi\|_{L^2}^2, \quad \Psi(t) := \|\mathbf{u}\|_{H^2}^2 + \|\partial_t \mathbf{u}\|_{L^2}^2 + \|\partial_t \varphi\|_{H^2}^2$$

- Strong (or regular) solutions** (full point-wise):

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Previous results

- **[Liu, DCDS'00]** Time-independent **[D1-D2]** B.C.:

Existence of global in time weak solutions.

Existence (and uniqueness) of global in time regular solutions for large viscosity ($\mu_4 \gg$), and its ω -limit is a nonempty set furnished by “equilibrium points”. Global minimizers of the elastic energy E_e are stable.

- **[Climent-Ezquerro & GG, CPAA'10]** Extension for time-dependent **[D1-D2]** B.C.

Moreover, Existence of time-periodic weak solutions and regularity for $\mu_4 \gg$.

- **[Segatti & Wu, SIMA'11]** Long-time behaviour with **periodic B.C.:**

Finite dimensional attractor in $2D$ domains.

Convergence to a single equilibrium (and convergence rate)

In particular, $\varphi(t) \rightarrow \varphi_\infty$ as $t \rightarrow \infty$, with $\frac{\delta E_e(\varphi_\infty)}{\delta \varphi} = 0$.

Moreover, local minimizers of the elastic energy E_e are stable.

RK: It may exist a “continuum” of equilibrium solutions with the same energy.

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Main result

Let S be the set of equilibrium points:

$$S = \{(0, \bar{\varphi}) : \bar{\varphi} \in H^4(\Omega), \Delta^2 \bar{\varphi} - \nabla \cdot \frac{1}{\varepsilon^2} \mathbf{f}(\bar{\varphi}) = 0, \bar{\varphi}|_{\partial\Omega} = \varphi_1, \partial_n \bar{\varphi}|_{\partial\Omega} = \varphi_2\}.$$

and the ω -limit set of a global weak solution:

$$\omega(\mathbf{u}, \varphi) = \{(\mathbf{u}_\infty, \varphi_\infty) \in \mathbf{V} \times \mathbf{H}^4 : \exists \{t_n\} \uparrow +\infty \text{ s.t. } (\mathbf{u}(t_n), \varphi(t_n)) \rightarrow (\mathbf{u}_\infty, \varphi_\infty) \text{ in } \mathbf{H}^1 \times \mathbf{H}^4\}.$$

Theorem

- $\omega(\mathbf{u}, \varphi) \subset S$
- $\omega(\mathbf{u}, \varphi) = \{(0, \varphi_\infty)\}$

Goal: Long-time behavior with admissible B.C.

Generic situation: Let $E(t), D(t) \geq 0$ satisfying the “**weak estimates**”:

$$(WE) \quad E'(t) + D(t) \leq 0, \quad \text{a.e. } t \in (0, +\infty).$$

Then, $E \in L^\infty(0, +\infty)$ and $E(t) \searrow E_\infty \geq 0$. Moreover, integrating (WE), one has $D \in L^1(0, +\infty)$.

Lemma ([Climent-Ezquerro, Rodriguez-Bellido & GG, JBC'10])

Let $D(t) \geq 0, D \in L^1(0, +\infty)$ satisfying the “**strong estimate**”:

$$(SE) \quad D'(t) \leq K(D(t)^3 + 1) \quad (K > 0).$$

Then, there exists $T^* \geq 0$ (large enough) such that $D \in L^\infty(T^*, +\infty)$ and

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Goal: Convergence uniformly with respect to the Galerkin sequence's index.

Theorem ([Climent-Ezquerro & GG, NA-TMA'14])

Let $E^m(t), D^m(t) \geq 0$, satisfying

$$(WE) \quad (E^m)'(t) + D^m(t) \leq 0,$$

$$(SE) \quad (D^m)'(t) \leq K(D^m(t)^3 + 1) \quad K > 0 \text{ independent of } m.$$

Then, $\forall \varepsilon < 1, \exists T^* = T^*(\varepsilon) \geq 0$ (large enough), *independent of m* , such that

$$\|D^m\|_{L^\infty(T^*, +\infty)} \leq \varepsilon.$$

Main steps to prove convergence to a single steady equilibrium

- ❶ To obtain (WE) and (SE) for $E(t) = E_{kin}(\mathbf{u}(t)) + \lambda E_e(\varphi(t))$ and

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- ❷ Existence of weak solutions (\mathbf{u}, φ) in $(0, +\infty)$ which are strong solutions in $(T_{reg}^*, +\infty)$ for some $T_{reg}^* > 0$.

- ❸ $E(\mathbf{u}(t), \varphi(t)) \searrow E_\infty$ in \mathbb{R} , $\mathbf{u}(t) \rightarrow 0$ in H_0^1 and $\frac{\delta E_e(\varphi(t))}{\delta \varphi} \rightarrow 0$ in L^2 (as $t \uparrow +\infty$).

- ❹ Recall the ω -limit set:

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Then, $\mathbf{u}_\infty = 0$ and $E_e(\varphi_\infty) = E_\infty$. Moreover:

- $\omega \neq \emptyset$.
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Theorem ("Strong" Łojasiewicz-Simon inequality for smectic-A problems)

If $\bar{\varphi} \in \mathcal{S}$, then there exists $C > 0$, $\beta > 0$ and $\theta \in (0, 1/2)$ depending on $\bar{\varphi}$ such that for all $\varphi \in H^4$ with $\varphi|_{\partial\Omega} = \varphi_1$, $\partial_n \varphi|_{\partial\Omega} = \varphi_2$ and $\|\varphi - \bar{\varphi}\|_{H^4} \leq \beta$, it holds

$$|E_e(\varphi) - E_e(\bar{\varphi})|^{1-\theta} \leq C \left\| \frac{\delta E_e(\varphi)}{\delta \varphi} \right\|_{L^2}$$

Proof: Application abstract result [S.Z. Huang, **Mathematical Surveys and Monographs**, vol. 126, AMS, 2006.]

Corollary ([Segatti, Wu, SIMA'11])

It's possible to relax the local hypothesis $\|\varphi - \bar{\varphi}\|_{H^4} \leq \beta$ by $\|\varphi - \bar{\varphi}\|_{H^3} \leq \tilde{\beta}$

Scheme: Finite Difference in time and Mixed Finite Element in space.

For simplicity,

- Uniform partition in time $t_n = nk$ of $[0, T]$ with $k = T/N$ (time step).
- inf-sup stable pair of FE for velocity-pressure.

Difficulties:

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Mixed second-order reformulation of (P)

By using the auxiliary variable $\psi = -\Delta\varphi$:

$$\left\{ \begin{array}{l} \left(\frac{D\mathbf{u}}{Dt}, \bar{\mathbf{u}} \right) + \left(\sigma^d, D(\bar{\mathbf{u}}) \right) - \left(\mathbf{p}, \nabla \cdot \bar{\mathbf{u}} \right) + \frac{\lambda}{\gamma} \left(\left(\frac{\partial \varphi}{\partial t} + \mathbf{u} \cdot \nabla \varphi \right) \nabla \varphi, \bar{\mathbf{u}} \right) = 0, \\ \left(\nabla \cdot \mathbf{u}, \bar{\mathbf{p}} \right) = 0, \\ \frac{\lambda}{\gamma} \left(\frac{\partial \varphi}{\partial t} + \mathbf{u} \cdot \nabla \varphi, \bar{\varphi} \right) + \lambda \left(\nabla \psi, \nabla \bar{\varphi} \right) + \frac{\lambda}{\varepsilon^2} \left(\mathbf{f}(\nabla \varphi), \nabla \bar{\varphi} \right) = 0 \\ \left(\partial_t \psi, \bar{\psi} \right) - \left(\nabla \partial_t \varphi, \nabla \bar{\psi} \right) = 0. \end{array} \right.$$

Energy law: Choosing $(\bar{\mathbf{u}}, \bar{\mathbf{p}}, \bar{\varphi}, \bar{\psi}) = (\mathbf{u}, \mathbf{p}, \partial_t \varphi, \lambda \psi)$

$$\frac{d}{dt} E_{tot}(\mathbf{u}, \psi, \nabla \varphi) + \left(\sigma^d, D(\mathbf{u}) \right) + \frac{\lambda}{\gamma} \left\| \frac{\partial \varphi}{\partial t} + \mathbf{u} \cdot \nabla \varphi \right\|_{L^2}^2 = 0,$$

where $E_{tot}(\mathbf{u}, \psi, \nabla \varphi) := E_{kin}(\mathbf{u}) + \lambda \left(E_{ela}(\psi) + E_{pen}(\nabla \varphi) \right)$,

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Generic second order scheme

Given $(\mathbf{u}^n, \varphi^n, \psi^n)$, compute $(\mathbf{u}^{n+1}, p^{n+\frac{1}{2}}, \varphi^{n+1}, \psi^{n+1}) \in \mathbf{U}_h \times P_h \times \Phi_h \times \Psi_h$ such that for any $(\bar{\mathbf{u}}, \bar{p}, \bar{\varphi}, \bar{\psi}) \in \mathbf{U}_h \times P_h \times \Phi_h \times \Psi_h$:

$$\begin{aligned} & \left(\delta_t \mathbf{u}^{n+1}, \bar{\mathbf{u}} \right) + c \left(\tilde{\mathbf{u}}, \mathbf{u}^{n+\frac{1}{2}}, \bar{\mathbf{u}} \right) + \left(\sigma^d(D(\mathbf{u}^{n+\frac{1}{2}}), \nabla \tilde{\varphi}), D(\bar{\mathbf{u}}) \right) \\ & - \left(p^{n+\frac{1}{2}}, \nabla \cdot \bar{\mathbf{u}} \right) + \frac{\lambda}{\gamma} \left((\delta_t \varphi^{n+1} + \mathbf{u}^{n+\frac{1}{2}} \cdot \nabla \tilde{\varphi}) \nabla \tilde{\varphi}, \bar{\mathbf{u}} \right) = 0, \\ & \left(\nabla \cdot \mathbf{u}^{n+\frac{1}{2}}, \bar{p} \right) = 0, \\ & \frac{\lambda}{\gamma} \left(\delta_t \varphi^{n+1} + \mathbf{u}^{n+\frac{1}{2}} \cdot \nabla \tilde{\varphi}, \bar{\varphi} \right) + \lambda \left(\nabla \psi^{n+\frac{1}{2}}, \nabla \bar{\varphi} \right) + \frac{\lambda}{\varepsilon^2} \left(\mathbf{f}^k(\nabla \varphi^{n+1}, \nabla \varphi^n), \nabla \bar{\varphi} \right) = 0, \\ & \left(\delta_t \psi^{n+1}, \bar{\psi} \right) - \left(\delta_t \nabla \varphi^{n+1}, \nabla \bar{\psi} \right) = 0 \end{aligned}$$

where $\mathbf{u}^{n+\frac{1}{2}} = (\mathbf{u}^{n+1} + \mathbf{u}^n)/2$ etc.

Lemma

The following discrete energy inequality holds:

$$\begin{aligned} & \delta_t E_{\text{tot}}(\mathbf{u}^{n+1}, \nabla \varphi^{n+1}, \mathbf{w}^{n+1}) + \mu_4 \|D(\mathbf{u}^{n+\frac{1}{2}})\|_{L^2(\Omega)}^2 \\ & + \frac{\lambda}{\gamma} \|\delta_t \varphi^{n+1} + \mathbf{u}^{n+\frac{1}{2}} \cdot \nabla \tilde{\varphi}\|_{L^2(\Omega)}^2 + \frac{\lambda}{\varepsilon^2} ND \leq 0, \end{aligned}$$

where

$$ND = \int_{\Omega} \mathbf{f}^k(\nabla \varphi^{n+1}, \nabla \varphi^n) \cdot \delta_t \nabla \varphi^{n+1} - \delta_t \left(\int_{\Omega} F(\nabla \varphi^{n+1}) \right).$$

Conclusions and open problems

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THANK YOU FOR YOUR ATTENTION